2-Pyrazoline, 3-ethyl-5-methyl

Inchi: InChI=1S/C6H12N2/c1-3-6-4-5(2)7-8-6/h5,7H,3-4H2,1-2H3
InchiKey: JGTXZZJCAVKRPL-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CCC1=NNC(C)C1
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
gf	261.01	kJ/mol	Joback Method
hf	48.40	kJ/mol	Joback Method
hfus	20.79	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.134		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	973.00		NIST Webbook
rinpol	973.00		NIST Webbook
tb	458.35	K	Joback Method
tc	679.67	K	Joback Method
tf	358.13	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.04	J/mol×K	458.35	Joback Method
cpg	230.63	J/mol×K	495.24	Joback Method
cpg	244.58	J/mol×K	532.12	Joback Method
cpg	257.87	J/mol×K	569.01	Joback Method
cpg	270.52	J/mol×K	605.89	Joback Method
cpg	282.50	J/mol×K	642.78	Joback Method
cpg	293.83	J/mol×K	679.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511165&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume